Effect of Surface Oxidation on Interfacial Water Structure at the Pyrite (100) Surface as Studied by MDS

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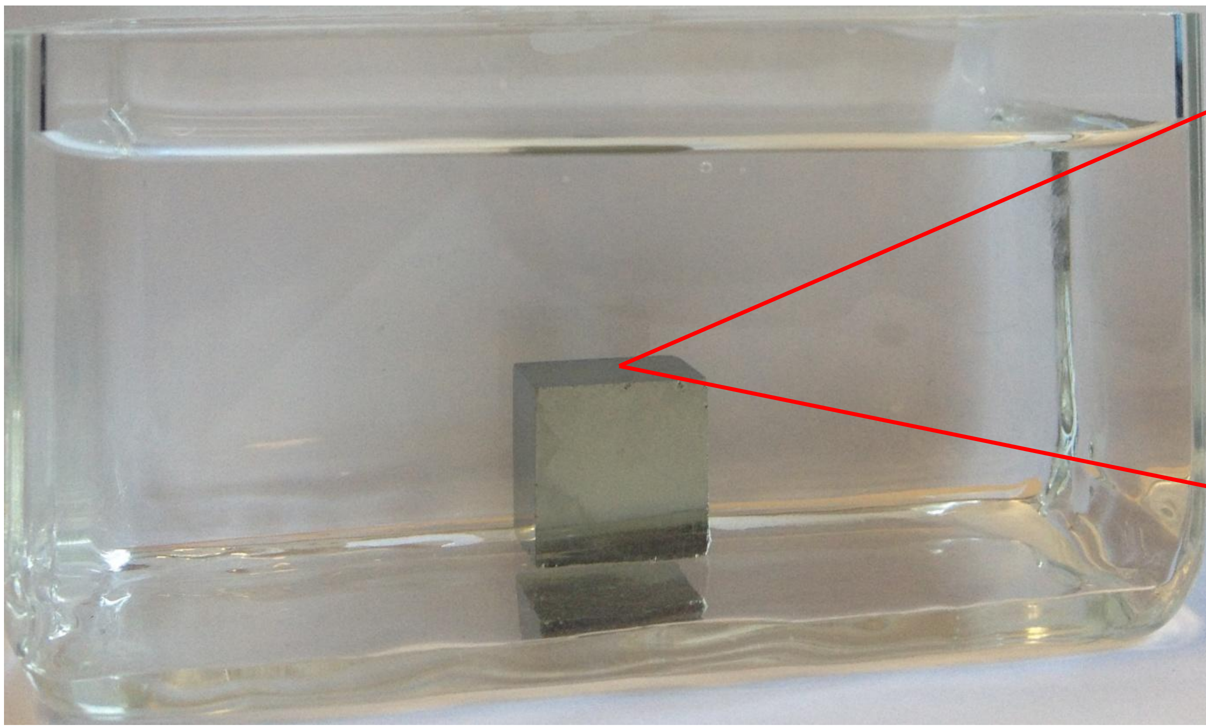
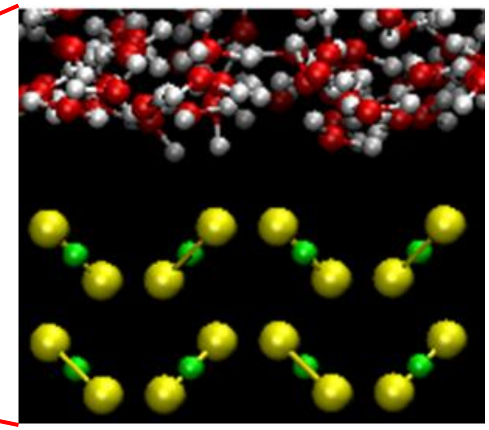


A cubic pyrite crystal soaked in water.

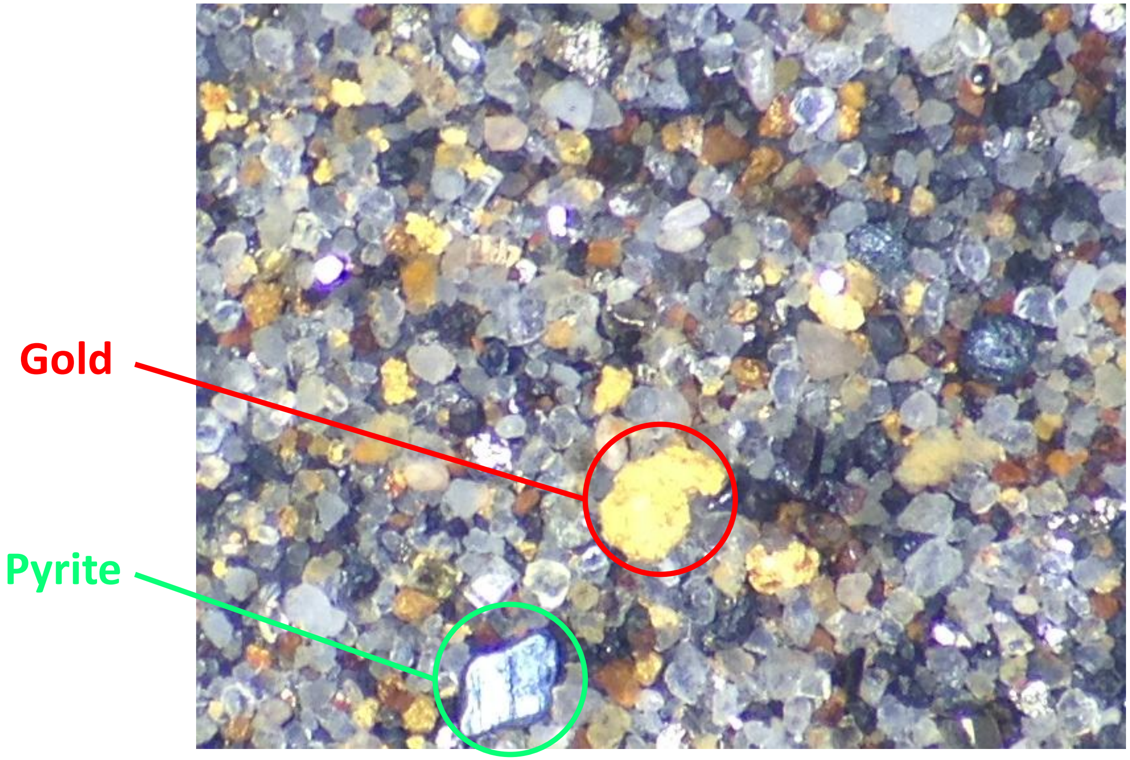


(Jin et al., 2014)

Flotation of Sulfide Minerals in Gold Production

Flotation provides a number of alternatives for the processing of gold ores containing sulfide minerals.

e.g. flotation of free gold and gold-bearing sulfides to produce a gold-rich concentrate for regrinding, oxidative pretreatment and cyanidation.



(*AngloGold Ashanti*).

Oxidation of Pyrite and Alteration of Its Surface Hydrophobicity

Pyrite is the most common host sulfide mineral for gold. Sulfide minerals are naturally hydrophobic under anaerobic conditions and have a natural floatability.

Generally the pyrite surfaces are oxidized under aerobic conditions and become hydrophilic.

Consequently, the flotation recovery of auriferous pyrite requires the use of collectors to create a hydrophobic surface state.

In this regard, the nature of the pyrite oxidized surface state should be examined in order to be able to establish collector adsorption reaction and the effective use of collector.

Oxidation of Pyrite Surface

The surface state of oxidized pyrite can include oxidation of iron and/or sulfur. The following possibilities have been identified for the pyrite surface:

Fresh unoxidized pyrite --- without and with $Fe(OH)^3$

Iron deficient polysulfide --- without and with $Fe(OH)^3$

Elemental sulfur --- without and with $Fe(OH)^3$

SEM and Contact Angle Measurement for Pyrite (100) Surface

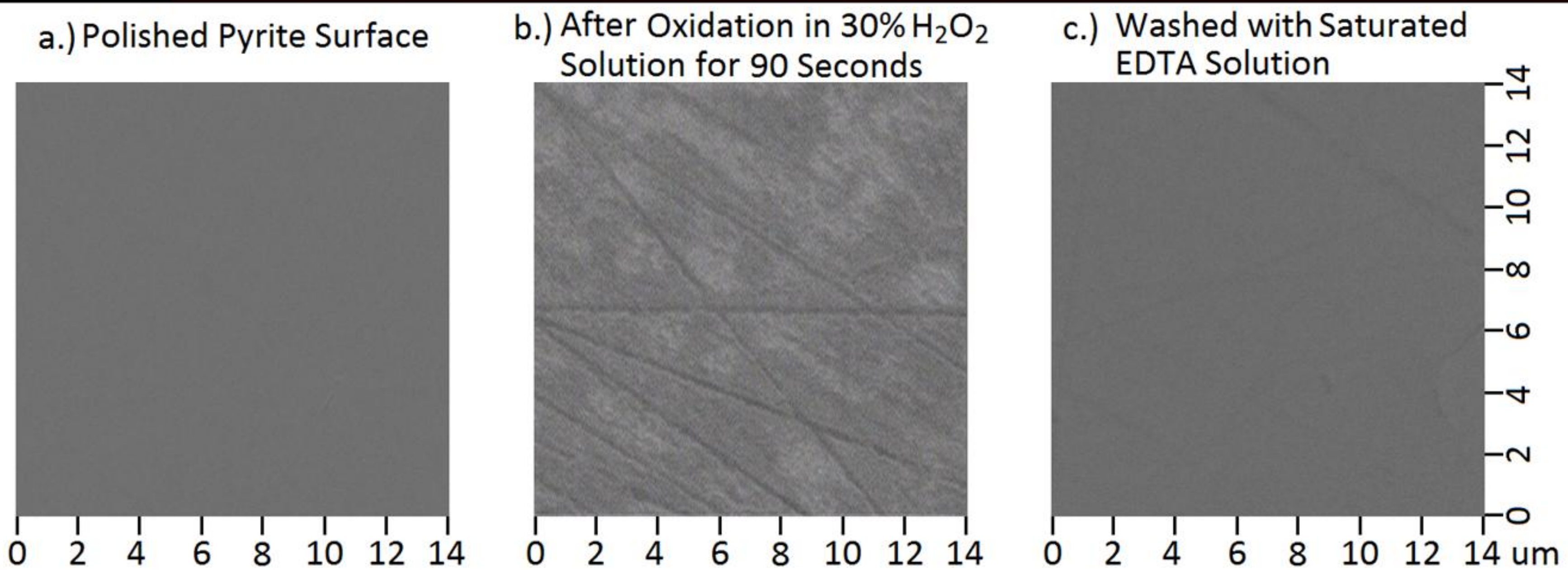


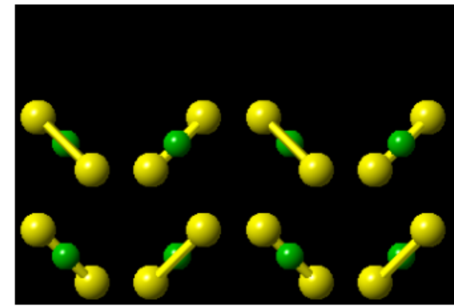
Figure 1. SEM images for pyrite (100) Surface

Table 1 Contact Angles for Pyrite (100) Surface

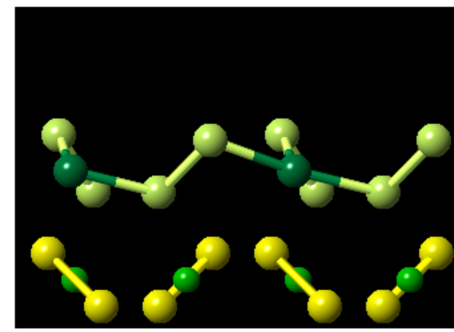
Pyrite (100) Surface	Contact Angle, Degree
After Polishing	62.5
Oxidized in 30% H2O2 Solution for 90 Seconds	23.0
Oxidized in 30% H2O2 Solution for 180 Seconds	12.0
Washed with EDTA Solution	64.5

Simulated Surfaces States Examined using MDS

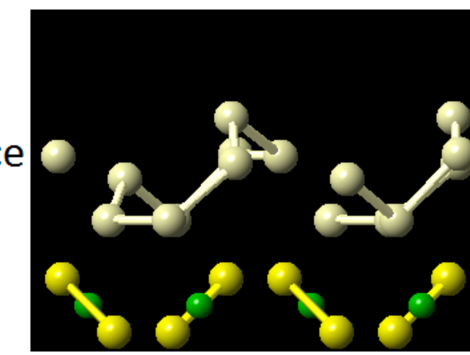
Fresh Pyrite (100) Surface — Fresh Unoxidized (100) Surface



Oxidized Pyrite (100) Surfaces
- Polysulfide at the (100) Surface



- Elemental Sulfur at the (100) Surface



(The atoms' color codes are as follow: yellow, S in pyrite crystal; green, Fe in pyrite crystal; dark green, Fe atoms in polysulfide; light green, S atoms in polysulfide; light yellow, elemental sulfur.)

Snapshots for Interfacial Water at Fresh Unoxidized (100) Surface of pyrite without/with Ferric Hydroxide

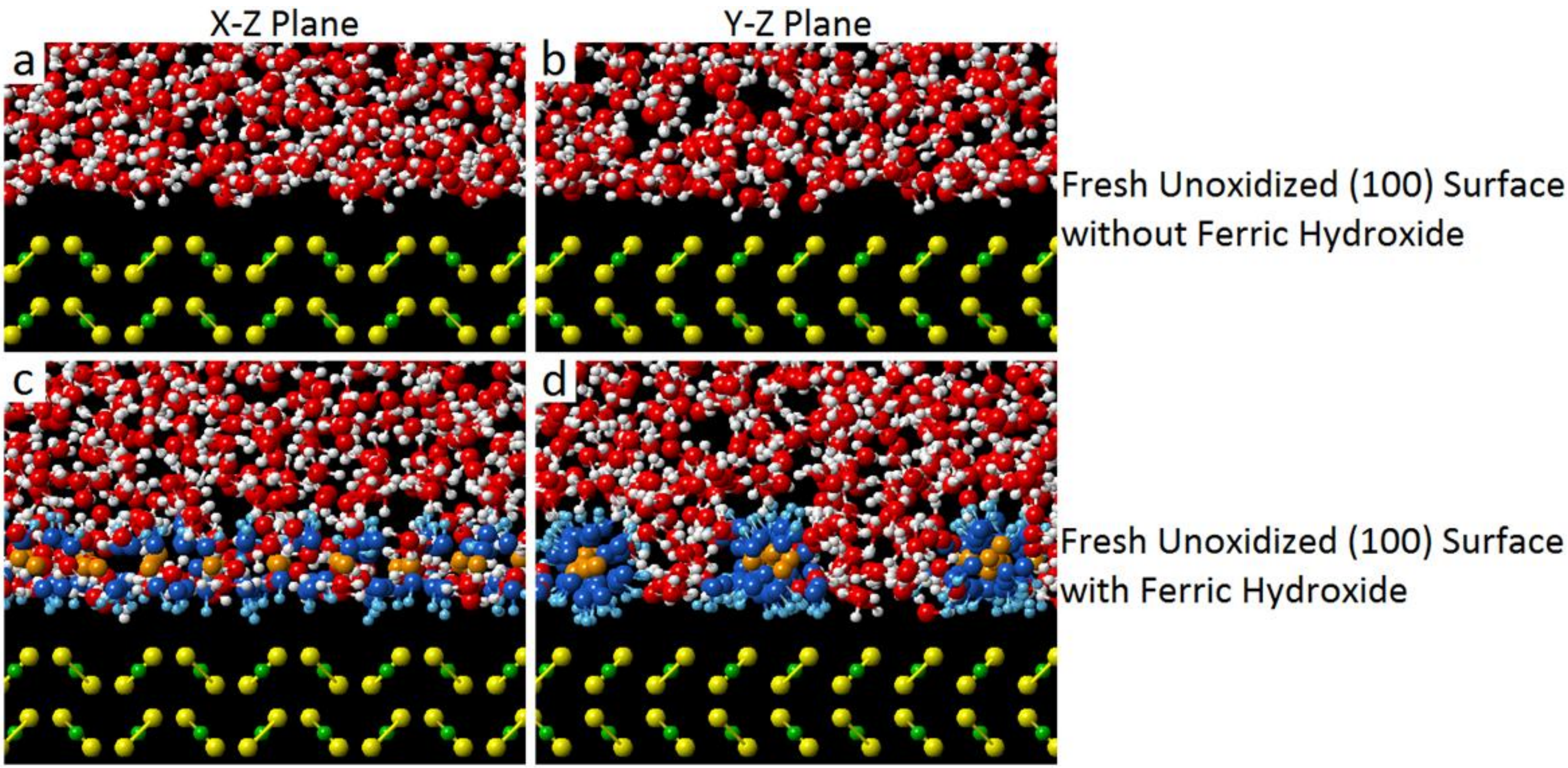


Figure 2. Snapshots for interfacial water at pyrite (100) surface. The atoms' color codes are as follow: red, O in water; white, H in water; blue, O in hydroxide; light blue, H in hydroxide; orange, $Fe3^{+}$ cations; yellow, S in pyrite crystal; green, Fe in pyrite crystal.

Snapshots for Interfacial Water at Polysulfide at the (100) Surface of pyrite without/with Ferric Hydroxide

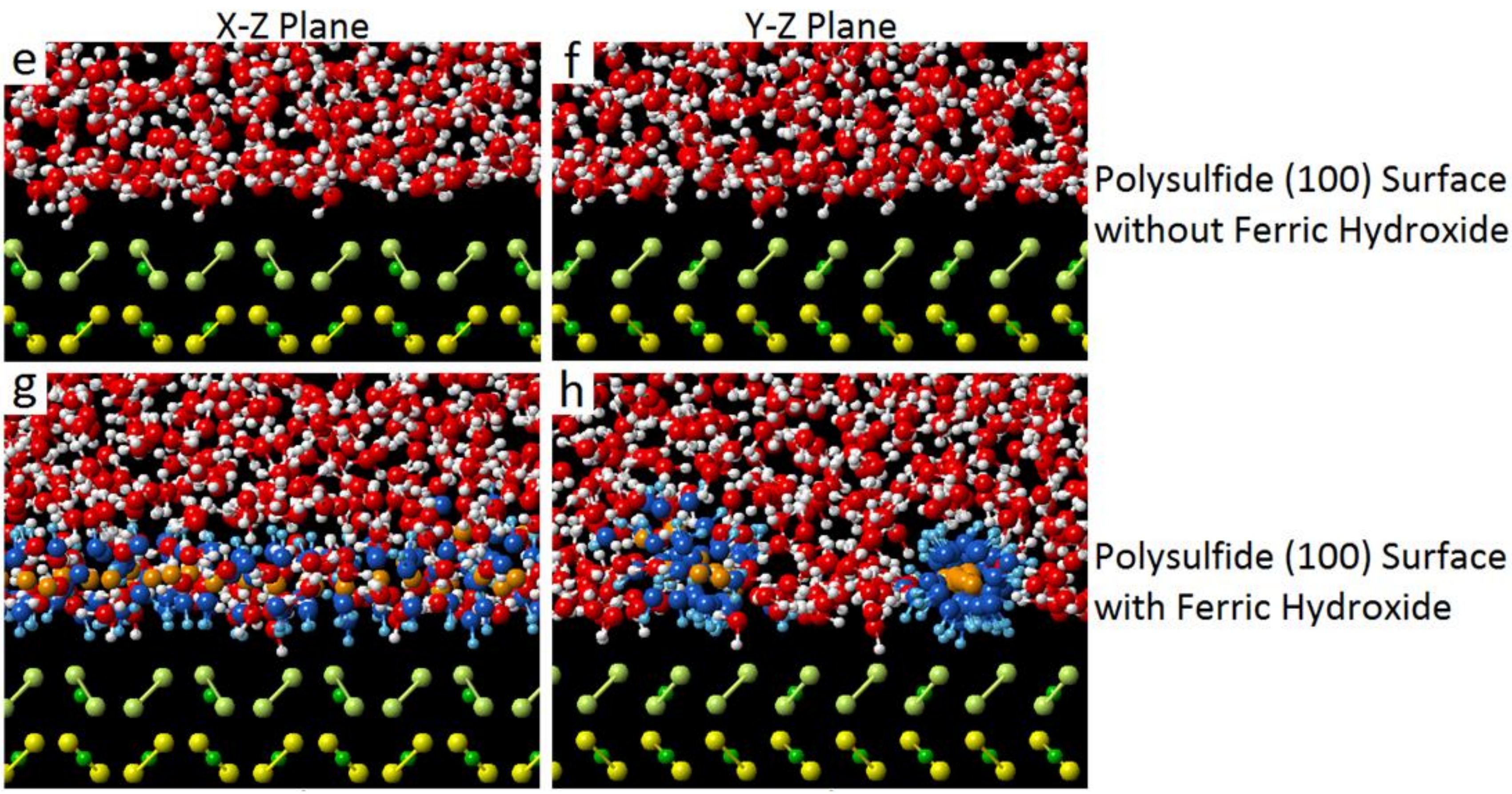
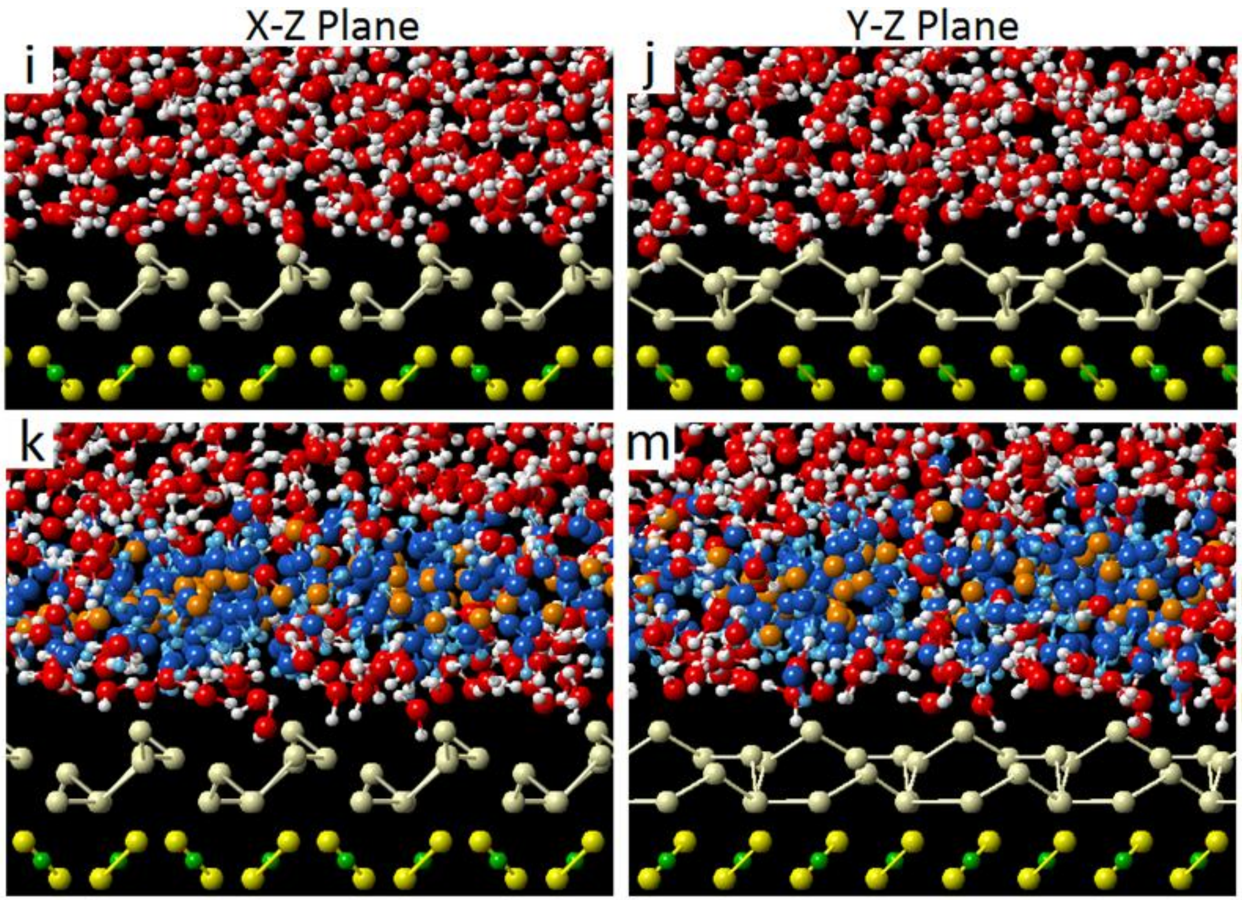


Figure 3. Snapshots for interfacial water at pyrite (100) surface. The atoms' color codes are as follow: red, O in water; white, H in water; blue, O in hydroxide; light blue, H in hydroxide; orange, $Fe3^{+}$ cations; yellow, S in pyrite crystal; green, Fe in pyrite or polysulfide; light green, S atoms in polysulfide.

Snapshots for Interfacial Water at Elemental Sulfur Rings at the (100) Surface of pyrite without/with Ferric Hydroxide



Elemental Sulfur 8-member Rings (100) Surface without Ferric Hydroxide

Elemental Sulfur 8-member Rings (100) Surface with Ferric Hydroxide

Figure 4. Snapshots for interfacial water at pyrite (100) surface. The atoms' color codes are as follow: red, O in water; white, H in water; blue, O in hydroxide; light blue, H in hydroxide; orange, $Fe3^{+}$ cations; yellow, S in pyrite crystal; green, Fe in pyrite crystal; light yellow, elemental sulfur.

Snapshots for a Water Drop at Fresh Unoxidized (100) Surface without/with Ferric Hydroxide

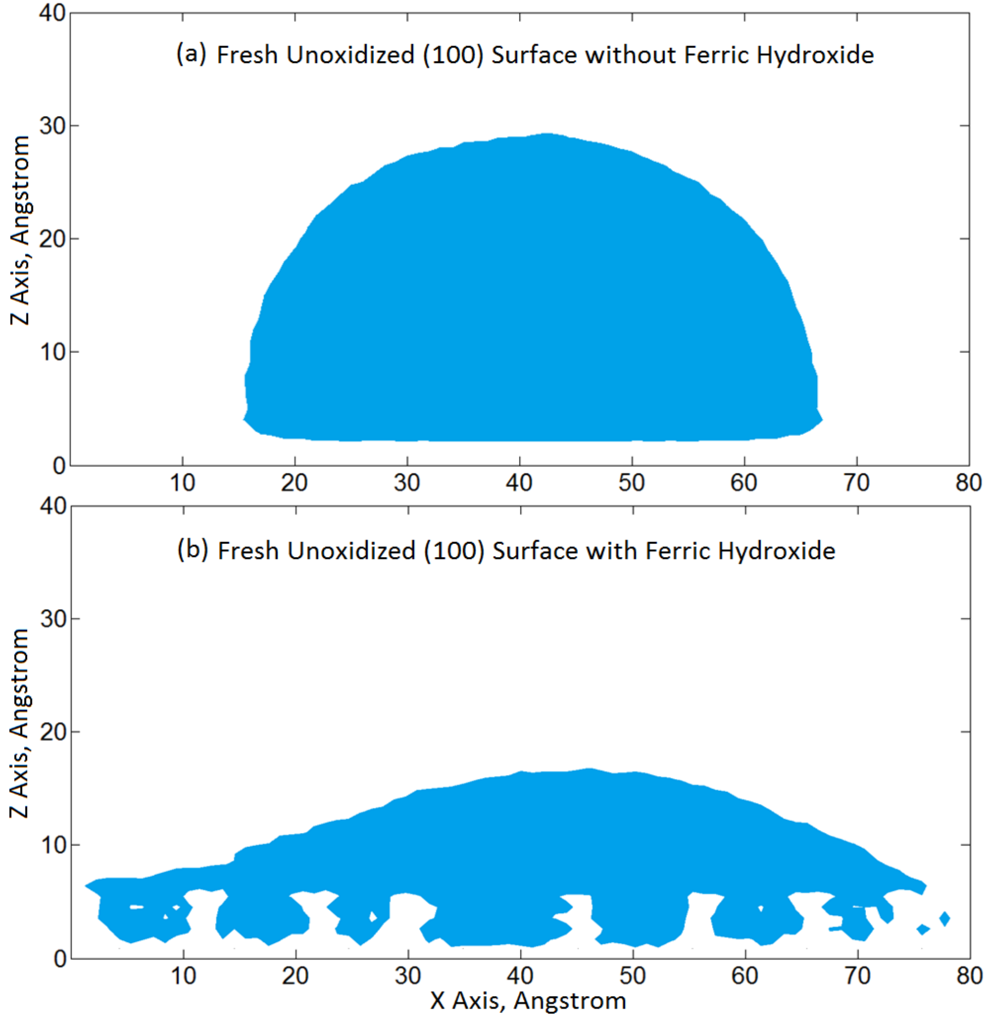


Figure 3. Water drop at fresh unoxidized pyrite (100) surface: (a) without ferric hydroxide; (b) with ferric hydroxide.

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Results for Simulated Contact Angle Measurements

Table 2 Simulated contact angles for pyrite (100) surface

Mineral Surface	Ferric Hydroxide	Contact Angle , Degree
Fresh Unoxidized (100) Surface	No	70.0
	Yes	24.0
Polysulfide at the (100) Surface	No	72.5
	Yes	22.0
Elemental Sulfur 8-member Rings at the (100) Surface	No	71.0
	Yes	14.0

The significance of the formation of ferric hydroxide islands in the corresponding hydrophilic surface state is revealed not only from experimental contact angle measurements but also from simulated contact angle measurements using MDS.

Water Residence Time Analysis

MDS reveals many features of the interfacial water structures, including water number density distribution, water dipole orientation, hydrogen bonds and water residence time.

For example, the interfacial water residence time appears to be the important indicator of the interfacial water. **The hydrophobic surface state will have a relatively small residence time, whereas the hydrophilic surface state is characterized by relatively larger residence time.**

Table 3 Water residence time for pyrite (100) surface

Mineral Surface	Ferric Hydroxide	Water Residence time , ps
Fresh Unoxidized (100) Surface	No	7.5
	Yes	17.2
Polysulfide at the (100) Surface	No	7.0
	Yes	14.0
Elemental Sulfur 8-member Rings at the (100) Surface	No	6.0
	Yes	18.6

Acknowledgements

References

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- Orlich, J., Gathje, J., Kappes, R., 2009. The application of froth flotation for gold recovery at Newmont Mining Corporation. Recent Advances in Mineral Processing Plant Design, 190.
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- Jin, J., Miller, J.D., Dang, L.X., Wick, C.D., 2014. Effect of surface oxidation on interfacial water structure at a pyrite (100) surface as studied by molecular dynamics simulation. International Journal of Mineral Processing (submitted in May 2014).